

On S -matrix of Schrödinger Operators with Non-Symmetric Zero-Range Potentials

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Abstract. Non-self-adjoint Schrödinger operators $A_{\mathfrak{T}}$ which correspond to non-symmetric zero-range potentials are investigated. We show that various properties of $A_{\mathfrak{T}}$ (eigenvalues, exceptional points, spectral singularities and the property of similarity to a self-adjoint operator) are completely determined by poles of the corresponding S -matrix.

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1. Introduction

This work was inspired by an intensive development of Pseudo-Hermitian Quantum Mechanics (PHQM) during last decades [1]. The key point of such theory is the employing of non-self-adjoint operators for the description of experimentally observable data. Briefly speaking, in order to interpret a given non-self-adjoint operator A in a Hilbert space \mathfrak{H} as a physically meaning Hamiltonian we have to check the reality of its spectrum and to prove the existence of a new inner product that ensures the (hidden) self-adjointness of A .

As usual, in PHQM studies, a non-self-adjoint operator A admits a representation $A = A_0 + V$, where A_0 is a fixed (unperturbed) self-adjoint operator in \mathfrak{H} and a non-symmetric potential V is characterized by a set $\Upsilon = \{\varepsilon\}$ of complex parameters ε . One of important problems is the description of quantitative and qualitative changes of spectrum $\sigma(A)$ when ε runs Υ . A typical evolution of properties is the following:

$$\begin{array}{ccccc}
 I & & II & & III \\
 \text{non-real} & \leftrightarrow & \text{spectral singularities} & \leftrightarrow & \text{similarity to} \\
 \text{eigenvalues} & & \text{exceptional points} & & \text{a self-adjoint operator}
 \end{array} \tag{1.1}$$

The properties of operators from domains I and III are quite obvious. In particular, the existence of non-real eigenvalues means that A cannot be realized as a self-adjoint operator for any choice of inner product. On the other hand, the similarity property shows that A turns out to be self-adjoint with respect to a new inner product of \mathfrak{H} which is equivalent to the initial one. The domain II can be interpreted as a boundary between I and III and the corresponding operators will keep only part of properties of I and III. For instance, if A corresponds to II, then its spectrum is real (similarly to III) but A cannot be made self-adjoint by an appropriate choice of equivalent inner product of \mathfrak{H} (in spirit of I). This phenomenon deals with the appearing of ‘wrong’ spectral points of A which are impossible for the spectra of self-adjoint operators. Traditionally, these spectral points are called *exceptional points* if they are located at the discrete spectrum of A and *spectral singularities* in the case of the continuous spectrum. Exceptional points correspond to situations where two or more eigenvalues together with their eigenvectors coalesce. Similar interpretation can also be carried out for spectral singularities with the use of generalized eigenvectors corresponding to the continuous spectrum. The presence of exceptional points/spectral singularities indicate that we lose the completeness of eigenvectors corresponding to eigenvalues and the continuous spectrum. Nowadays, various aspects of exceptional points/spectral singularities including the physical meaning and possible practical applications has been analyzed with a wealth of technical tools (see, e.g., [2] for exceptional points and [3] for spectral singularities).

In the present paper, we show that the evolution of spectral properties (1.1) can be successfully and easily described in terms of poles of S -matrices of operators A . We illustrate this point by considering the set of operators A generated by the Schrödinger

type differential expression $A = -\frac{d^2}{dx^2} + V$ with zero-range potential

$$V = a < \delta, \cdot > \delta(x) + b < \delta', \cdot > \delta(x) + c < \delta, \cdot > \delta'(x) + d < \delta', \cdot > \delta'(x),$$

where δ and δ' are, respectively, the Dirac δ -function and its derivative and a, b, c, d are complex numbers.

The Schrödinger operator with zero-range potential fits well the Lax-Phillips scattering scheme [4] since the potential is concentrated at one point (so-called 0-perturbations [5]). In that case the S -matrix (the Lax-Phillips scattering matrix) of A coincides with the meromorphic matrix-valued function

$$S(k) = [\sigma_0 - 2(1 - ik)\mathfrak{T}][\sigma_0 - 2(1 + ik)\mathfrak{T}]^{-1}, \quad k \in \mathbb{C}, \quad \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.2)$$

where (2×2) -matrix \mathfrak{T} is expressed in terms of parameters a, b, c, d and it determines the domain of definition of A (see (2.6)). If the matrix \mathfrak{T} is *Hermitian*, then the corresponding operator $A = A_{\mathfrak{T}}$ is self-adjoint and the S -matrix (1.2) is the direct consequence of mathematically rigorous arguments of scattering theory: establishing the existence of wave operators with subsequent representation of the scattering operator in the spectral representation of unperturbed dynamics [6].

In the case of a non-self-adjoint operator $A_{\mathfrak{T}}$ we define the S -matrix by analogy, considering *an arbitrary matrix* \mathfrak{T} in (1.2) and do not take care about auxiliary mathematical things (see [7], [8] for details). We found this definition useful because: a) the formula (1.2) for S -matrix enables to determine explicitly the matrix \mathfrak{T} characterizing the operator $A_{\mathfrak{T}}$; b) the formula (1.2) can be easily rewritten in terms of right/left reflection and transmission coefficients of the corresponding traveling wave functions (cf. subsection 2.4).

The Lax-Phillips scattering scheme allows to define S -matrices for Schrödinger operators with local (i.e., the support of potential is a bounded interval) non-symmetric potentials. The obtained formulas are similar to (1.2) and they also can be rewritten via reflection/transmission coefficients [8]. We believe that such an interpretation of S -matrix which comes from the Lax-Phillips scattering theory makes it possible to establish more informative connection between poles of S -matrix and spectral properties of Schrödinger operators with local non-symmetric potentials.

In this paper, using the decomposition of the S -matrix (1.2) with respect to the Pauli matrices (subsection 2.3), we show that the location of poles of the S -matrix $S(\cdot)$ completely determines the spectral properties of non-self-adjoint operators $A_{\mathfrak{T}}$ outlined in (1.1).

Our proof of similarity of $A_{\mathfrak{T}}$ to a self-adjoint operator in section 3 does not contain an algorithm of the construction of an appropriate metric operator e^Q which guarantees the self-adjointness of $A_{\mathfrak{T}}$. However, in the particular case where the S -matrix of a non-self-adjoint operator $A_{\mathfrak{T}}$ has simple imaginary poles, we ‘guess’ an explicit expression of the metric operator (section 4). Sections 5 and 6 are devoted to spectral singularities and exceptional points, respectively.

Throughout the paper $\mathcal{D}(A)$ denotes the domain and $\ker A$ denotes the null-space of a linear operator A . The resolvent set and the spectrum of A are denoted by $\rho(A)$ and $\sigma(A)$, respectively.

2. Schrödinger operator with non-symmetric zero-range potentials

2.1. Preliminaries

A one-dimensional Schrödinger operator with general zero-range potential at the point $x = 0$ can be defined by the formal expression

$$-\frac{d^2}{dx^2} + a < \delta, \cdot > \delta(x) + b < \delta', \cdot > \delta(x) + c < \delta, \cdot > \delta'(x) + d < \delta', \cdot > \delta'(x), \quad (2.1)$$

where δ and δ' are, respectively, the Dirac δ -function and its derivative (with support at 0) and a, b, c, d are complex numbers. Using the regularization method suggested in [9], a direct relationship between parameters a, b, c, d of the singular potential

$$V = a < \delta, \cdot > \delta(x) + b < \delta', \cdot > \delta(x) + c < \delta, \cdot > \delta'(x) + d < \delta', \cdot > \delta'(x) \quad (2.2)$$

and operator-realizations of (2.1) in the Hilbert space $L_2(\mathbb{R})$ can be established [10]. Precisely, the formal expression (2.1) gives rise to operators

$$A_{\mathbf{T}} = -\frac{d^2}{dx^2}, \quad \mathbf{T} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \quad (2.3)$$

defined on smooth functions $f \in W_2^2(\mathbb{R} \setminus \{0\})$ which satisfy the boundary condition

$$\mathbf{T} \begin{pmatrix} \frac{f(0+) + f(0-)}{2} \\ \frac{-f'(0+) - f'(0-)}{2} \end{pmatrix} = \begin{pmatrix} f'(0+) - f'(0-) \\ f(0+) - f(0-) \end{pmatrix}. \quad (2.4)$$

Remark 2.1. The matrix \mathbf{T} in (2.4) relates the mean values of functions f, f' at point 0 with their jumps. Another description of point interaction at point 0 can be given by the matching conditions

$$\mathbf{B} \begin{pmatrix} f(0-) \\ f'(0-) \end{pmatrix} = \begin{pmatrix} f(0+) \\ f'(0+) \end{pmatrix} \quad (2.5)$$

which connect the left-side and the right-side boundary values of the functions f, f' at point 0 [11]. The sets of operators defined via the boundary conditions (2.4) and (2.5)

do not coincide. For instance, the operator $A_{\mathbf{T}}$ with $\mathbf{T} = \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix}$ cannot be realized with the use of (2.5).

2.2. Definition and elementary properties of S -matrix

The S -matrix $S(\cdot)$ of $A_{\mathbf{T}}$ can be directly expressed in terms of \mathbf{T} since the potential V is supported at point 0. However, the obtained formula looks quite cumbersome. Having in mind to simplify the expression for $S(\cdot)$, we rewrite the boundary condition (2.4) in the form

$$\mathfrak{T} \begin{pmatrix} f(0+) + f'(0+) \\ f(0-) - f'(0-) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} f(0+) \\ f(0-) \end{pmatrix}, \quad \mathfrak{T} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}. \quad (2.6)$$

It should be noted that the set of operators $A_{\mathfrak{T}} = -\frac{d^2}{dx^2}$ determined by the boundary condition (2.6) does not coincide with the set of operators $A_{\mathbf{T}}$ defined by (2.3), (2.4). Namely, the domain of definition of $A_{\mathbf{T}}$ admits the presentation (2.6) if and only -1 does not belong to the point spectrum of $A_{\mathbf{T}}$ or, that is equivalent (see [12]), if

$$\Xi = 4 - \det \mathbf{T} + 2(a - d) \neq 0, \quad \det \mathbf{T} = ad - bc. \quad (2.7)$$

In that case, it is easy to verify by comparing (2.4) and (2.6) that

$$\mathfrak{T} = \frac{1}{4\Xi} \begin{pmatrix} \Xi + 2(b + c - a - d) & 4 + \det \mathbf{T} - 2(b - c) \\ 4 + \det \mathbf{T} + 2(b - c) & \Xi - 2(b + c + a + d) \end{pmatrix}. \quad (2.8)$$

On the other hand, not every operator $A_{\mathfrak{T}}$ can be rewritten as $A_{\mathbf{T}}$ (for example $A_{\mathfrak{T}}$ with $\mathfrak{T} = 0$ does not belong to the set of operators $A_{\mathbf{T}}$).

The operators $A_{\mathfrak{T}}$ fit well the Lax-Phillips scattering scheme and the corresponding S -matrix of $A_{\mathfrak{T}}$ coincides with the matrix-valued function

$$S(k) = [\sigma_0 - 2(1 - ik)\mathfrak{T}][\sigma_0 - 2(1 + ik)\mathfrak{T}]^{-1}, \quad \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (2.9)$$

determined for all $k \in \mathbb{C}_+ = \{k \in \mathbb{C} : \operatorname{Im} k > 0\}$ where (2.9) is well posed [7], [8].

The expression (2.9) enables to determine the S -matrix $S(\cdot)$ of $A_{\mathfrak{T}}$ for any (2×2) -matrix \mathfrak{T} . In the particular case where \mathfrak{T} admits the representation (2.8) (i.e., the matrix \mathfrak{T} can be expressed via \mathbf{T} and hence, $A_{\mathfrak{T}} \equiv A_{\mathbf{T}}$) we will say that $S(\cdot)$ is the S -matrix of $A_{\mathbf{T}}$.

Remark 2.2. (i) In the Lax-Phillips scattering scheme the free evolution is determined by the Friedrichs extension of the symmetric operator

$$A_s = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_s) = \left\{ f \in W_2^2(\mathbb{R} \setminus \{0\}) : \begin{array}{l} f(0+) = f(0-) = 0 \\ f'(0+) = f'(0-) = 0 \end{array} \right\} \quad (2.10)$$

associated with given differential expression (2.1). Namely, the Friedrichs extension coincides with the operator

$$A_F = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_F) = \{f \in W_2^2(\mathbb{R} \setminus \{0\}) : f(0+) = f(0-) = 0\}. \quad (2.11)$$

The self-adjoint operator A_F is determined by $\mathfrak{T} = 0$ in (2.6). Thus, the matrix \mathfrak{T} characterizes ‘a deviation’ of $A_{\mathfrak{T}}$ from the unperturbed Hamiltonian A_F . In some sense, this explains why the matrix \mathfrak{T} (rather than \mathbf{T}) appears in (2.9).

(ii) The self-adjoint operator

$$A_K = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_K) = \{f \in W_2^2(\mathbb{R} \setminus \{0\}) : f'(0+) = f'(0-) = 0\} \quad (2.12)$$

is determined by $\mathfrak{T} = \frac{1}{2}\sigma_0$ in (2.6) and it is the Krein extension of the symmetric operator A_s . Similarly to the Friedrichs extension A_F , the Krein extension A_K determines a free evolution in the Lax-Phillips scattering scheme [13]. The corresponding S -matrices are: $S(k) = \sigma_0$ for A_F and $S(k) = -\sigma_0$ for A_K .

(iii) The expression (2.9) determines the S -matrix for $A_{\mathbf{T}}$ only in the case where $-1 \in \rho(A_{\mathbf{T}})$. It turns out that the formula (2.9) and the results below can be easily modified for any operator $A_{\mathbf{T}}$ with nonempty resolvent set.

It follows from (2.9) that the S -matrix $S(\cdot)$ is a meromorphic matrix-function on \mathbb{C}_+ . It can be established that poles of $S(\cdot)$ correspond to eigenvalues of $A_{\mathfrak{T}}$. Precisely, $k \in \mathbb{C}_+$ is a pole of $S(\cdot)$ if and only if k^2 is an eigenvalue of $A_{\mathfrak{T}}$ [12]. The formula (2.9) allows to extend the definition of S -matrix of $A_{\mathfrak{T}}$ to all complex numbers $k \in \mathbb{C}$ satisfying the condition $\det[\sigma_0 - 2(1 + ik)\mathfrak{T}] \neq 0$. Obviously, the extended S -matrix remains to be a meromorphic matrix-function.

We will say that $S(\cdot)$ has a pole at infinity if at least one of entries of $S(k)$ tend to infinity when $k \rightarrow \infty$. We will say that $S(k)$ is defined on the *physical sheet* if $k \in \mathbb{C}_+$ and $S(k)$ is defined on the *nonphysical sheet* if $k \in \mathbb{C}_- = \{k \in \mathbb{C} : \text{Im } k < 0\}$.

According to the above discussion the discrete spectrum of $A_{\mathfrak{T}}$ is completely determined by the corresponding S -matrix on the physical sheet \mathbb{C}_+ .

2.3. The presentations of S -matrix with the use of Pauli matrices

The S -matrix for a non-self-adjoint operator $A_{\mathfrak{T}}$ may have new unusual properties. For this reason, an additional representations of $S(\cdot)$ can be useful. First of all, we are interesting in the decomposition of $S(\cdot)$ with respect to the Pauli matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Let X be an arbitrary (2×2) -matrix. Then X admits the presentation $X = \sum_{j=0}^3 x_j \sigma_j$, where $x_j \in \mathbb{C}$. In that case

$$\det X = x_0^2 - \sum_{j=1}^3 x_j^2 \quad \text{and} \quad X^{-1} = \frac{1}{\det X} \left(x_0 \sigma_0 - \sum_{j=1}^3 x_j \sigma_j \right). \quad (2.13)$$

In particular, if $X = \sigma_0 - 2(1 + ik)\mathfrak{T}$, then

$$\det[\sigma_0 - 2(1 + ik)\mathfrak{T}] = 4(1 + ik)^2 \det \mathfrak{T} - 4(1 + ik)\gamma_0 + 1 \quad (2.14)$$

and

$$[\sigma_0 - 2(1 + ik)\mathfrak{T}]^{-1} = \frac{(1 - 2(1 + ik)\gamma_0)\sigma_0 + 2(1 + ik) \sum_{j=1}^3 \gamma_j \sigma_j}{4(1 + ik)^2 \det \mathfrak{T} - 4(1 + ik)\gamma_0 + 1}, \quad (2.15)$$

where $\gamma_j \in \mathbb{C}$ are determined uniquely by the decomposition

$$\mathfrak{T} = \sum_{j=0}^3 \gamma_j \sigma_j, \quad \text{and} \quad \mathbf{det} \mathfrak{T} = \gamma_0^2 - \sum_{j=1}^3 \gamma_j^2.$$

Substituting (2.15) into (2.9) and making elementary calculations we obtain another representation of S -matrix of $A_{\mathfrak{T}}$

$$S(k) = \sigma_0 + 4ik \frac{\mathfrak{T} - 2(1+ik)\mathbf{det} \mathfrak{T} \sigma_0}{4(1+ik)^2 \mathbf{det} \mathfrak{T} - 4(1+ik)\gamma_0 + 1}. \quad (2.16)$$

The general formula (2.16) can be simplified if we will consider separately the cases $\mathbf{det} \mathfrak{T} \neq 0$ and $\mathbf{det} \mathfrak{T} = 0$. Denote $\theta_k = 2(1+ik)$ and assume that $\mathbf{det} \mathfrak{T} \neq 0$. Then

$$4(1+ik)^2 \mathbf{det} \mathfrak{T} - 4(1+ik)\gamma_0 + 1 = \frac{(\theta_k - \theta_+)(\theta_k - \theta_-)}{\theta_- \theta_+}, \quad (2.17)$$

where

$$\theta_+ = \frac{1}{\gamma_0 + \sqrt{\sum_{j=1}^3 \gamma_j^2}}, \quad \theta_- = \frac{1}{\gamma_0 - \sqrt{\sum_{j=1}^3 \gamma_j^2}}, \quad \mathbf{det} \mathfrak{T} = \frac{1}{\theta_- \theta_+}. \quad (2.18)$$

Therefore, (2.16) can be rewritten as

$$S(k) = \sigma_0 + 4ik \frac{\theta_- \theta_+ \mathfrak{T} - \theta_k \sigma_0}{(\theta_k - \theta_+)(\theta_k - \theta_-)}. \quad (2.19)$$

The decomposition of $S(k)$ with respect to the Pauli matrices has the form

$$S(k) = \sum_{j=0}^3 s_j(k) \sigma_j, \quad (2.20)$$

where

$$s_0(k) = 1 + 4ik \frac{\theta_- \theta_+ \gamma_0 - \theta_k}{(\theta_k - \theta_+)(\theta_k - \theta_-)}, \quad s_j(k) = 4ik \frac{\theta_- \theta_+ \gamma_j}{(\theta_k - \theta_+)(\theta_k - \theta_-)}, \quad j \geq 1. \quad (2.21)$$

Let $\mathbf{det} \mathfrak{T} = 0$. Then at least one of θ_{\pm} is equal to ∞ and (2.19) is reduced to

$$S(k) = \sigma_0 + \frac{4ik}{1 - 2\theta_k \gamma_0} \mathfrak{T}. \quad (2.22)$$

Sometimes it is useful to calculate the S -matrix directly in terms of coefficients a, b, c, d of the initial singular potential (2.2). This means that we consider the particular case where $A_{\mathfrak{T}} \equiv A_{\mathbf{T}}$ and \mathfrak{T} is defined by (2.8). In that case the coefficients γ_j of the decomposition $\mathfrak{T} = \sum_{j=0}^3 \gamma_j \sigma_j$ have the form

$$\begin{aligned} \gamma_0 &= \frac{1}{4\Xi} (\Xi - 2(a+d)), & \gamma_1 &= \frac{1}{4\Xi} (4 + \mathbf{det} \mathbf{T}), \\ \gamma_2 &= \frac{-i}{2\Xi} (b-c), & \gamma_3 &= \frac{1}{2\Xi} (b+c), \end{aligned} \quad (2.23)$$

where $\Xi = 4 - \mathbf{det} \mathbf{T} + 2(a-d)$. Furthermore, the identities

$$\mathbf{det} \mathfrak{T} = -\frac{d}{2\Xi}, \quad \sum_{j=1}^3 \gamma_j^2 = \frac{(4 + \mathbf{det} \mathbf{T})^2 + 16bc}{16\Xi^2} \quad (2.24)$$

are deduced directly from (2.8) and (2.23). (We remind that Ξ is always non-zero due to our assumption $-1 \in \rho(A_{\mathbf{T}})$, see (2.7).) Substituting the obtained relations into (2.16) we obtain the expression of $\mathbf{S}(\cdot)$ in terms of the coefficients a, b, c, d . In particular, if $d = 0$, then $\det \mathfrak{T} = 0$ and the expression (2.16) is reduced to

$$\mathbf{S}(k) = \sigma_0 + \frac{4ik\Xi}{2a(1+ik) - ik\Xi} \mathfrak{T}. \quad (2.25)$$

Example I. *δ -potential with a complex coupling.* Let $a \in \mathbb{C}$ and $b = c = d = 0$. Then (2.1) takes the form

$$-\frac{d^2}{dx^2} + a < \delta, \cdot > \delta(x), \quad a \in \mathbb{C}$$

and (2.4) determines the operators $A_{\mathbf{T}} \equiv A_a = -\frac{d^2}{dx^2}$ with domains of definition

$$\mathcal{D}(A_a) = \left\{ f \in W_2^2(\mathbb{R} \setminus \{0\}) \mid \begin{array}{l} f(0+) = f(0-) \ (\equiv f(0)) \\ f'(0+) - f'(0-) = af(0) \end{array} \right\}.$$

The matrix \mathfrak{T} in (2.8) and Ξ are

$$\mathfrak{T} = \frac{1}{4+2a} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \Xi = 4 + 2a.$$

By virtue of (2.25),

$$\mathbf{S}(k) = \frac{1}{2k+ia} \begin{pmatrix} ia & -2k \\ -2k & ia \end{pmatrix}.$$

Example II. *Mixed complex δ -potential.* Let $b \in \mathbb{C}$ and $a = c = d = 0$. Then (2.1) is reduced to

$$-\frac{d^2}{dx^2} + b < \delta', \cdot > \delta(x), \quad b \in \mathbb{C}$$

and domains of definition the corresponding operators $A_{\mathbf{T}} \equiv A_b = -\frac{d^2}{dx^2}$ take the form

$$\mathcal{D}(A_b) = \left\{ f \in W_2^2(\mathbb{R} \setminus \{0\}) \mid \begin{array}{l} f(0+) = f(0-) \ (\equiv f(0)) \\ (2+b)f'(0+) = (2-b)f'(0-) \end{array} \right\}.$$

The matrix \mathfrak{T} and Ξ are

$$\mathfrak{T} = \frac{1}{8} \begin{pmatrix} 2+b & 2-b \\ 2+b & 2-b \end{pmatrix}, \quad \Xi = 4.$$

Using (2.25) again we obtain

$$\mathbf{S}(k) = \frac{-1}{2} \begin{pmatrix} b & 2-b \\ 2+b & -b \end{pmatrix}.$$

Example III. *The case where the S -matrix is a constant on \mathbb{C} .* The S -matrices of operators A_b in Example II do not depend on k and they are constants on \mathbb{C} .

Let $A_{\mathfrak{T}}$ be an operator defined by (2.6) and let $S_{\mathfrak{T}}(\cdot)$ be the corresponding S -matrix. An elementary analysis of (2.19), (2.21), and (2.22) shows that $S_{\mathfrak{T}}(k)$ does not depend on $k \in \mathbb{C}$ if and only if $\mathfrak{T} = 0$, $\mathfrak{T} = \frac{1}{2}\sigma_0$, or

$$\mathfrak{T} = \frac{1}{4}\sigma_0 + \sum_{j=1}^3 \gamma_j \sigma_j, \quad \text{where} \quad \sum_{j=1}^3 \gamma_j^2 = \frac{1}{16}.$$

In these cases, respectively,

$$S_0(k) = \sigma_0, \quad S_{\frac{1}{2}\sigma_0}(k) = -\sigma_0, \quad S_{\mathfrak{T}}(k) = -4 \sum_{j=1}^3 \gamma_j \sigma_j.$$

Assume now that the matrix \mathfrak{T} can be expressed via \mathbf{T} and hence, $A_{\mathfrak{T}} \equiv A_{\mathbf{T}}$. Using, (2.23), (2.24), and (2.25), we conclude that the S -matrix $S_{\mathbf{T}}(k)$ of $A_{\mathbf{T}}$ is a constant on \mathbb{C} if and only if $a = d = 0$.

2.4. The presentation of S -matrix in terms of transmission and reflection coefficients

The expression (2.9) of the S -matrix was obtained within the framework of the Lax-Phillips scattering theory and, certainly, it looks quite unusual. Our aim now is to rewrite (2.9) in terms of transmission and reflection coefficients of the wave functions

$$f_1 = \begin{cases} e^{-i\bar{k}x} + R_k^r e^{ikx}, & x > 0 \\ T_k^r e^{-ikx}, & x < 0 \end{cases}, \quad f_2 = \begin{cases} T_k^l e^{ikx}, & x > 0 \\ e^{ikx} + R_k^l e^{-ikx}, & x < 0 \end{cases} \quad (2.26)$$

where $k \in \mathbb{C}' = \mathbb{C} \setminus i\mathbb{R} = \{k \in \mathbb{C} : \operatorname{Re} k \neq 0\}$.

It follows from (2.26) that:

$$\begin{aligned} f_1(0+) &= 1 + R_k^r, & f_1(0-) &= T_k^r, & f_1'(0+) &= i(-\bar{k} + kR_k^r), & f_1'(0-) &= -ikT_k^r, \\ f_2(0+) &= T_k^l, & f_2(0-) &= 1 + R_k^l, & f_2'(0+) &= ikT_k^l, & f_2'(0-) &= i(\bar{k} - kR_k^l). \end{aligned}$$

Substituting these values in (2.6) and solving the corresponding systems of linear equations, we get

$$\begin{aligned} t_{11} &= \frac{1}{\theta_k \Delta_k} [\Delta_k - (e^{i\alpha} - 1)(R_k^l + e^{i\alpha})], & t_{12} &= \frac{T_k^l}{\theta_k \Delta_k} (e^{i\alpha} - 1), \\ t_{22} &= \frac{1}{\theta_k \Delta_k} [\Delta_k - (e^{i\alpha} - 1)(R_k^r + e^{i\alpha})], & t_{21} &= \frac{T_k^r}{\theta_k \Delta_k} (e^{i\alpha} - 1), \end{aligned}$$

where $\theta_k = 2(1 + ik)$, $e^{i\alpha} = \frac{\bar{\theta}_k}{\theta_k}$, $k \in \mathbb{C}'_+$, and

$$\Delta_k = \begin{vmatrix} R_k^r + e^{i\alpha}, & T_k^r \\ T_k^l, & R_k^l + e^{i\alpha} \end{vmatrix}.$$

Then

$$\sigma_0 - 2(1 + ik)\mathfrak{T} = \frac{e^{i\alpha} - 1}{\Delta_k} \begin{pmatrix} R_k^l + e^{i\alpha} & -T_k^l \\ -T_k^r & R_k^r + e^{i\alpha} \end{pmatrix}$$

and

$$\det[\sigma_0 - 2(1 + ik)\mathfrak{T}] = \frac{(e^{i\alpha} - 1)^2}{\Delta_k}.$$

Hence,

$$[\sigma_0 - 2(1 + ik)\mathfrak{T}]^{-1} = \frac{1}{e^{i\alpha} - 1} \begin{pmatrix} R_k^r + e^{i\alpha} & T_k^l \\ T_k^r & R_k^l + e^{i\alpha} \end{pmatrix}. \quad (2.27)$$

Rewriting (2.9) as

$$S(k) = \frac{1 - ik}{1 + ik} \sigma_0 + \frac{2ik}{1 + ik} [\delta_0 - 2(1 + ik)\mathfrak{T}]^{-1}, \quad k \in \mathbb{C}'_+,$$

using (2.27), and taking into account that

$$\frac{2ik}{1 + ik} \cdot \frac{1}{e^{i\alpha} - 1} = -\frac{k}{\operatorname{Re} k}, \quad \frac{1 - ik}{1 + ik} - \frac{k}{\operatorname{Re} k} e^{i\alpha} = -i \frac{\operatorname{Im} k}{\operatorname{Re} k}$$

we obtain

$$S(k) = -\frac{k}{\operatorname{Re} k} \begin{pmatrix} R_k^r + i \frac{\operatorname{Im} k}{k} & T_k^l \\ T_k^r & R_k^l + i \frac{\operatorname{Im} k}{k} \end{pmatrix}. \quad (2.28)$$

The expression (2.28) coincides with the S -matrix of $A_{\mathfrak{T}}$ for all $k \in \mathbb{C}'$ such that

$$\Delta_k = \begin{vmatrix} R_k^r + e^{i\alpha}, & T_k^r \\ T_k^l, & R_k^l + e^{i\alpha} \end{vmatrix} \neq 0, \quad e^{i\alpha} = \frac{1 - i\bar{k}}{1 + ik}.$$

3. Similarity to self-adjoint operators

An operator A acting in a Hilbert space \mathfrak{H} is called *similar* to a self-adjoint operator H if there exists a bounded and boundedly invertible operator Z such that

$$A = Z^{-1} H Z. \quad (3.1)$$

It is known (see, for example, [14]) that *the similarity of A to a self-adjoint operator means that A is self-adjoint for a certain choice of inner product of the Hilbert space \mathfrak{H} , which is equivalent to the initial inner product (\cdot, \cdot) .*

The following integral-resolvent criterion of similarity can be useful:

Lemma 3.1 ([15]). *A closed densely defined operator A acting in \mathfrak{H} is similar to a self-adjoint one if and only if the spectrum of A is real and there exists a constant M such that*

$$\begin{aligned} \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|(A - zI)^{-1} g\|^2 d\xi &\leq M \|g\|^2, \\ \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|(A^* - zI)^{-1} g\|^2 d\xi &\leq M \|g\|^2, \quad \forall g \in \mathfrak{H}, \end{aligned} \quad (3.2)$$

where the integrals are taken along the line $z = \xi + i\varepsilon$ ($\varepsilon > 0$ is fixed) of \mathbb{C}_+ .

In order to use Lemma 3.1 we need an explicit form of the resolvent $(A_{\mathfrak{T}} - zI)^{-1}$.

Lemma 3.2. *Let $A_{\mathfrak{T}}$ and A_F be linear operators in $L_2(\mathbb{R})$ defined, respectively, by (2.6) and (2.11). Then, for all $g \in L_2(\mathbb{R})$ and for all $z = k^2$ ($k \in \mathbb{C}_+$) from the resolvent set of $A_{\mathfrak{T}}$*

$$\|[(A_{\mathfrak{T}} - zI)^{-1} - (A_F - zI)^{-1}]g\|^2 = \frac{1}{\operatorname{Im} k} \left\| \frac{(\sigma_0 + i\sigma_2)[\mathfrak{T} - \theta_k \mathbf{det} \mathfrak{T} \sigma_0]}{p_{\mathfrak{T}}(k)} Fg \right\|_{\mathbb{C}^2}^2,$$

where $\theta_k = 2(1 + ik)$, $\|\cdot\|_{\mathbb{C}^2}$ is the norm in \mathbb{C}^2 , $Fg = \begin{pmatrix} \int_0^\infty e^{iks} g(s) ds \\ \int_{-\infty}^0 e^{-iks} g(s) ds \end{pmatrix}$ and

$$p_{\mathfrak{T}}(k) = 4(1 + ik)^2 \mathbf{det} \mathfrak{T} - 4(1 + ik)\gamma_0 + 1. \quad (3.3)$$

Proof. Let us fix $k \in \mathbb{C}_+$ and consider the functions

$$h_{1k}(x) = \begin{cases} e^{ikx}, & x > 0 \\ e^{-ikx}, & x < 0 \end{cases} \quad h_{2k}(x) = \begin{cases} -e^{ikx}, & x > 0 \\ e^{-ikx}, & x < 0 \end{cases} \quad (3.4)$$

which belong $L_2(\mathbb{R})$ and form a basis of $\ker(A_s^* - zI)$, where $z = k^2 \in \mathbb{C} \setminus \mathbb{R}_+$ and A_s^* is the adjoint of the symmetric operator A_s defined by (2.10). Similarly to the proof of Lemma 4 in [10], we conclude that

$$[(A_{\mathfrak{T}} - zI)^{-1} - (A_F - zI)^{-1}]g = c_{1k}h_{1k} + c_{2k}h_{2k}, \quad \forall g \in L_2(\mathbb{R}), \quad (3.5)$$

where c_{jk} are two parameters to be calculated. The latter relation allows one to express any function $f \in \mathcal{D}(A_{\mathfrak{T}})$ as follows:

$$f(x) = f_F(x) + c_{1k}h_{1k}(x) + c_{2k}h_{2k}(x), \quad (3.6)$$

where $f_F = (A_F - zI)^{-1}g \in \mathcal{D}(A_F)$ and $f_F(0+) = f_F(0-) = 0$ (in view of (2.11)).

The functions f in (3.6) satisfy (2.6). Calculating the values of $f(0\pm)$, $f'(0\pm)$ with the help of (3.4) and (3.6), substituting them to (2.6) and making elementary transformations we get

$$\begin{pmatrix} c_{1k} \\ c_{2k} \end{pmatrix} = (\sigma_0 + i\sigma_2)\mathfrak{T}(\sigma_0 - \theta_k \mathfrak{T})^{-1} \begin{pmatrix} f'_F(0+) \\ -f'_F(0-) \end{pmatrix}. \quad (3.7)$$

Simple calculation with the use of (2.15) and properties of Pauli matrices gives

$$(\sigma_0 + i\sigma_2)\mathfrak{T}(\sigma_0 - \theta_k \mathfrak{T})^{-1} = \frac{(\sigma_0 + i\sigma_2)[\mathfrak{T} - \theta_k \mathbf{det} \mathfrak{T} \sigma_0]}{p_{\mathfrak{T}}(k)}.$$

On the other hand, taking into account the explicit expression of $(A_F - zI)^{-1}$:

$$(A_F - zI)^{-1}g = \begin{cases} \frac{e^{ikx}}{k} \int_0^x g(s) \sin ksd s + \frac{\sin kx}{k} \int_x^\infty e^{iks} g(s) ds, & x > 0; \\ -\frac{e^{-ikx}}{k} \int_x^0 g(s) \sin ksd s - \frac{\sin kx}{k} \int_{-\infty}^x e^{-iks} g(s) ds, & x < 0 \end{cases}$$

we obtain

$$\begin{pmatrix} f'_F(0+) \\ -f'_F(0-) \end{pmatrix} = \begin{pmatrix} \int_0^\infty e^{iks} g(s) ds \\ \int_{-\infty}^0 e^{-iks} g(s) ds \end{pmatrix}.$$

Thus, (3.7) can be rewritten as

$$\begin{pmatrix} c_{1k} \\ c_{2k} \end{pmatrix} = \frac{(\sigma_0 + i\sigma_2)[\mathfrak{T} - \theta_k \mathbf{det} \mathfrak{T}\sigma_0]}{p_{\mathfrak{T}}(k)} Fg, \quad \text{where} \quad Fg = \begin{pmatrix} \int_0^\infty e^{iks} g(s) ds \\ \int_{-\infty}^0 e^{-iks} g(s) ds \end{pmatrix}.$$

The functions h_{jk} in (3.4) are orthogonal in $L_2(\mathbb{R})$ and $\|h_{jk}\|^2 = \frac{1}{\operatorname{Im} k}$. Hence, (3.5) gives

$$\|[(A_{\mathfrak{T}} - zI)^{-1} - (A_F - zI)^{-1}]g\|^2 = \frac{|c_{1k}|^2 + |c_{2k}|^2}{\operatorname{Im} k} = \frac{1}{\operatorname{Im} k} \left\| \frac{(\sigma_0 + i\sigma_2)[\mathfrak{T} - \theta_k \mathbf{det} \mathfrak{T}\sigma_0]}{p_{\mathfrak{T}}(k)} Fg \right\|_{\mathbb{C}^2}^2$$

that completes the proof of Lemma 3.2 ■

Theorem 3.3. *If all poles of the S-matrix $S(\cdot)$ of $A_{\mathfrak{T}}$ lie on the nonphysical sheet \mathbb{C}_- , then $A_{\mathfrak{T}}$ is similar to a self-adjoint operator.*

Proof. The operator A_F defined by (2.11) is self-adjoint. Hence, it satisfies (3.2) and the inequalities

$$\begin{aligned} \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|[(A_{\mathfrak{T}} - zI)^{-1} - (A_F - zI)^{-1}]g\|^2 d\xi &\leq M\|g\|^2, \\ \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|[(A_{\mathfrak{T}}^* - zI)^{-1} - (A_F - zI)^{-1}]g\|^2 d\xi &\leq M\|g\|^2, \quad \forall g \in L_2(\mathbb{R}), \end{aligned} \quad (3.8)$$

give us the necessarily and sufficient condition for the similarity of $A_{\mathfrak{T}}$ to a self-adjoint operator.

Firstly we consider the auxiliary self-adjoint operator A_K defined by (2.12). Obviously, the inequalities (3.8) are true with $A_{\mathfrak{T}} = A_K$. Using Lemma 3.2, and taking into account that

$$A_K = A_{\frac{1}{2}\sigma_0}, \quad \mathbf{det} \frac{1}{2}\sigma_0 = \frac{1}{4}, \quad p_{\frac{1}{2}\sigma_0}(k) = -k^2$$

we get

$$\|[(A_K - zI)^{-1} - (A_F - zI)^{-1}]g\|^2 = \frac{1}{\operatorname{Im} k} \left\| \frac{(\sigma_0 + i\sigma_2)}{2k} Fg \right\|_{\mathbb{C}^2}^2.$$

Therefore, in view of (3.8),

$$\int_{-\infty}^{\infty} \frac{\varepsilon}{\operatorname{Im} k} \left\| \frac{(\sigma_0 + i\sigma_2)}{k} Fg \right\|_{\mathbb{C}^2}^2 d\xi \leq M\|g\|^2. \quad (3.9)$$

We note that the integral in (3.9) is taken along the line $z = k^2 = \xi + i\varepsilon$ ($\varepsilon > 0$ is fixed) of upper half-plane \mathbb{C}_+ . This means that

$$\varepsilon = 2(\operatorname{Re} k)(\operatorname{Im} k) > 0, \quad \xi = (\operatorname{Re} k)^2 - (\operatorname{Im} k)^2.$$

Therefore, the variable k belongs to $\mathbb{C}_{++} = \{k \in \mathbb{C}_+ : \operatorname{Re} k > 0\}$ when $k^2 = \xi + i\varepsilon$.

Let $A_{\mathfrak{T}}$ be an operator defined by (2.6). Assume that the S -matrix of $A_{\mathfrak{T}}$ has poles on the nonphysical sheet \mathbb{C}_- only. Then, taking into account (2.16) and (2.21), we conclude that the roots of $p_{\mathfrak{T}}(k)$ belong to \mathbb{C}_- . Hence, the entries of the matrix

$$\Psi(k) = \frac{k}{p_{\mathfrak{T}}(k)} [\mathfrak{T} - \theta_k \mathbf{det} \mathfrak{T}\sigma_0]$$

are uniformly bounded when k runs \mathbb{C}_{++} . Taking in mind this fact, Lemma 3.2 and (3.9) we obtain

$$\varepsilon \int_{-\infty}^{\infty} \|[(A_{\mathfrak{T}} - zI)^{-1} - (A_F - zI)^{-1}]g\|^2 d\xi = \int_{-\infty}^{\infty} \frac{\varepsilon}{\operatorname{Im} k} \left\| \frac{(\sigma_0 + i\sigma_2)}{k} \Psi(k) Fg \right\|_{\mathbb{C}^2}^2 d\xi \leq$$

$$M_1 \int_{-\infty}^{\infty} \frac{\varepsilon}{\operatorname{Im} k} \left\| \frac{(\sigma_0 + i\sigma_2)}{k} Fg \right\|_{\mathbb{C}^2}^2 d\xi < MM_1 \|g\|^2$$

that establish the first inequality in (3.8).

The second inequality can be justified in a similar manner. Indeed, it is easy to check that the domain of definition $\mathcal{D}(A_{\mathfrak{T}}^*)$ has the form (2.6) with \mathfrak{T}^* (instead of \mathfrak{T}). Thus,

$$A_{\mathfrak{T}}^* = A_{\mathfrak{T}^*}. \quad (3.10)$$

Let $S_{\mathfrak{T}}(\cdot)$ and $S_{\mathfrak{T}^*}(\cdot)$ be the S -matrix of operators $A_{\mathfrak{T}}$ and $A_{\mathfrak{T}^*}$, respectively. It follows from (2.9) that

$$S_{\mathfrak{T}^*}(-\bar{k}) = S_{\mathfrak{T}}^*(k), \quad k \in \mathbb{C}. \quad (3.11)$$

Therefore, the S -matrix of $A_{\mathfrak{T}^*}$ also has poles within \mathbb{C}_- . This allows one to establish the second relation in (3.8) by repeating the previous arguments with the use of modified matrix

$$\Psi(k) = \frac{k}{p_{\mathfrak{T}^*}(k)} [\mathfrak{T}^* - \theta_k \mathbf{det} \mathfrak{T}^* \sigma_0].$$

In view of Lemma 3.1 and inequalities (3.8) the operator $A_{\mathfrak{T}}$ is similar to a self-adjoint one. Theorem 3.3 is proved. ■

Corollary 3.4. *Let the S -matrix of $A_{\mathfrak{T}}$ be a constant on \mathbb{C} (see Example III). Then $A_{\mathfrak{T}}$ is similar to a self-adjoint operator.*

4. Metric operators

Unfortunately, the proof of Theorem 3.3 does not contain ‘a recipe’ of construction of an appropriate metric operator which guarantees the self-adjointness of $A_{\mathfrak{T}}$. We just state that such an operator exists. Various approaches to the explicit determination of metric operator with the use of formal perturbative methods as well as mathematically rigid constructions can be found in [16].

In this section we are aiming to find an explicit expression for metric operators in the case where the S -matrix $S(\cdot)$ of $A_{\mathfrak{T}}$ has simple non-zero imaginary poles.

Assume that Q is a self-adjoint operator in $L_2(\mathbb{R})$. Then $e^{\chi Q}$, ($\chi \in \mathbb{R}$) is a positive self-adjoint operator in $L_2(\mathbb{R})$. If there exists a metric operator $e^{\chi Q}$ such that

$$e^{\chi Q} A_{\mathfrak{T}} = A_{\mathfrak{T}}^* e^{\chi Q}, \quad (4.1)$$

then $A_{\mathfrak{T}}$ turns out to be self-adjoint with respect to the new inner product $\|\cdot\|_{new}^2 = (e^{\chi Q} \cdot, \cdot) = \|e^{\chi Q/2} \cdot\|^2$ of $L_2(\mathbb{R})$.

Using (3.10) we rewrite (4.1) in the equivalent form

$$e^{\chi Q} A_{\mathfrak{T}} = A_{\mathfrak{T}^*} e^{\chi Q} \quad (4.2)$$

and we will seek the operator Q in (4.2) as:

$$Q_{\vec{\alpha}} = \alpha_1 \mathcal{P} + \alpha_2 i \mathcal{P} \mathcal{R} + \alpha_3 \mathcal{R}, \quad \vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{S}^2, \quad (4.3)$$

where $\mathbb{S}^2 = \{\vec{\alpha} \in \mathbb{R}^3 : \sum_{j=1}^3 \alpha_j^2 = 1\}$ and

$$\mathcal{P}f(x) = f(-x), \quad \mathcal{R}f(x) = (\operatorname{sgn} x)f(x), \quad \forall f \in L_2(\mathbb{R}) \quad (4.4)$$

are self-adjoint operators in $L_2(\mathbb{R})$.

The operators $Q_{\vec{\alpha}}$ are self-adjoint in $L_2(\mathbb{R})$ and $Q_{\vec{\alpha}}^2 = I$ [7]. Therefore,

$$e^{\chi Q_{\vec{\alpha}}} = (\cosh \chi)I + (\sinh \chi)Q_{\vec{\alpha}}, \quad \chi \in \mathbb{R}. \quad (4.5)$$

It follows from (4.3) – (4.5) that $e^{\chi Q_{\vec{\alpha}}}$ commutes with the operator

$$A_s^* = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_s^*) = W_2^2(\mathbb{R} \setminus \{0\}).$$

Since $A_{\mathfrak{T}}$ and $A_{\mathfrak{T}^*}$ are restrictions of A_s^* , respectively, onto $\mathcal{D}(A_{\mathfrak{T}})$ and $\mathcal{D}(A_{\mathfrak{T}^*})$ the relation (4.2) holds if and only if the operator $e^{\chi Q_{\vec{\alpha}}}$ maps $\mathcal{D}(A_{\mathfrak{T}})$ into $\mathcal{D}(A_{\mathfrak{T}^*})$, Taking (2.6) into account we conclude that the relation $e^{\chi Q_{\vec{\alpha}}} : \mathcal{D}(A_{\mathfrak{T}}) \rightarrow \mathcal{D}(A_{\mathfrak{T}^*})$ is equivalent to the following implication

$$\text{if } \mathfrak{T}\Gamma_0 f = \Gamma_1 f, \quad \text{then } \mathfrak{T}^* \Gamma_0 e^{\chi Q_{\vec{\alpha}}} f = \Gamma_1 e^{\chi Q_{\vec{\alpha}}} f, \quad \forall f \in \mathcal{D}(A_{\mathfrak{T}}), \quad (4.6)$$

$$\text{where } \Gamma_0 f = \begin{pmatrix} f(0+) + f'(0+) \\ f(0-) - f'(0-) \end{pmatrix} \quad \text{and} \quad \Gamma_1 f = \frac{1}{2} \begin{pmatrix} f(0+) \\ f(0-) \end{pmatrix}.$$

It is easily to check, using the definition (4.4) of operators \mathcal{P} and \mathcal{R} , that

$$\Gamma_k \mathcal{P}f = \sigma_1 \Gamma_k f, \quad \Gamma_k \mathcal{R}f = \sigma_3 \Gamma_k f, \quad \Gamma_k i \mathcal{P} \mathcal{R}f = i \sigma_1 \sigma_3 \Gamma_k f = \sigma_2 \Gamma_k f, \quad \forall f \in W_2^2(\mathbb{R} \setminus \{0\}).$$

Therefore, $\Gamma_k e^{\chi Q_{\vec{\alpha}}} f = (\cosh \chi \sigma_0 + \sinh \chi \sigma_{\vec{\alpha}}) \Gamma_k f$, $k = 0, 1$, where $\sigma_{\vec{\alpha}} = \sum_{j=1}^3 \alpha_j \sigma_j$ and implication (4.6) is equivalent to equation

$$\mathfrak{T}^* (\cosh \chi \sigma_0 + \sinh \chi \sigma_{\vec{\alpha}}) = (\cosh \chi \sigma_0 + \sinh \chi \sigma_{\vec{\alpha}}) \mathfrak{T} \quad (4.7)$$

with respect to unknown $\chi \in \mathbb{R}$ and $\vec{\alpha} \in \mathbb{S}^2$.

Assume that all poles of S -matrix $\mathbf{S}(\cdot)$ of a *non-self-adjoint operator* $A_{\mathfrak{T}}$ are simple and they belong to $\mathbb{R} \setminus \{0\}$. In view of (2.18) – (2.22), the case of *two different simple non-zero imaginary poles* of $\mathbf{S}(\cdot)$ is characterized by the conditions

$$\det \mathfrak{T} \neq 0, \quad \gamma_0 \in \mathbb{R}, \quad \sqrt{\sum_{j=1}^3 \gamma_j^2} \in \mathbb{R} \setminus \{0\}, \quad (4.8)$$

where (as usual) $\mathfrak{T} = \sum_{j=0}^3 \gamma_j \sigma_j$. Similarly the case where S -matrix of a non-self-adjoint operator $A_{\mathfrak{T}}$ has *one simple non-zero imaginary pole* corresponds to the relations

$$\det \mathfrak{T} = 0, \quad \gamma_0 \in \mathbb{R}, \quad \sqrt{\sum_{j=1}^3 \gamma_j^2} \in \mathbb{R} \setminus \{0\}. \quad (4.9)$$

The condition $\gamma_0 \in \mathbb{R}$ in both cases (4.8) and (4.9) allows to rewrite the equation (4.7) as follows:

$$\sum_{j=1}^3 (\operatorname{Im} \gamma_j) \sigma_j = \tanh \chi \left(\begin{vmatrix} \sigma_1 & \sigma_2 & \sigma_3 \\ \operatorname{Re} \gamma_1 & \operatorname{Re} \gamma_2 & \operatorname{Re} \gamma_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{vmatrix} - \sum_{j=1}^3 (\operatorname{Im} \gamma_j) \alpha_j \sigma_0 \right), \quad (4.10)$$

where the formal determinant

$$\begin{vmatrix} \sigma_1 & \sigma_2 & \sigma_3 \\ \operatorname{Re} \gamma_1 & \operatorname{Re} \gamma_2 & \operatorname{Re} \gamma_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{vmatrix} := \begin{vmatrix} \operatorname{Re} \gamma_2 & \operatorname{Re} \gamma_3 \\ \alpha_2 & \alpha_3 \end{vmatrix} \sigma_1 - \begin{vmatrix} \operatorname{Re} \gamma_1 & \operatorname{Re} \gamma_3 \\ \alpha_1 & \alpha_3 \end{vmatrix} \sigma_2 + \begin{vmatrix} \operatorname{Re} \gamma_1 & \operatorname{Re} \gamma_2 \\ \alpha_1 & \alpha_2 \end{vmatrix} \sigma_3$$

is the ‘cross product’ of vectors $\operatorname{Re} \vec{\gamma} = (\operatorname{Re} \gamma_1, \operatorname{Re} \gamma_2, \operatorname{Re} \gamma_3)$ and $\vec{\alpha}$ which is associated with the Pauli matrices $\sigma_1, \sigma_2, \sigma_3$ (instead of the standard basis vectors $\mathbf{i}, \mathbf{j}, \mathbf{k}$ of the Euclidean space \mathbb{R}^3).

We remark that the vectors

$$\operatorname{Re} \vec{\gamma} = (\operatorname{Re} \gamma_1, \operatorname{Re} \gamma_2, \operatorname{Re} \gamma_3), \quad \operatorname{Im} \vec{\gamma} = (\operatorname{Im} \gamma_1, \operatorname{Im} \gamma_2, \operatorname{Im} \gamma_3)$$

in (4.10) cannot be zero. Indeed, if $\operatorname{Re} \vec{\gamma} = \vec{0}$, then $\sqrt{\sum_{j=1}^3 \gamma_j^2} = \sqrt{-\sum_{j=1}^3 |\gamma_j|^2} \in i\mathbb{R} \setminus \{0\}$ that contradicts to the third relation in (4.8), (4.9). Similarly, if $\operatorname{Im} \vec{\gamma} = \vec{0}$, then the second relation in (4.8), (4.9) implies that $A_{\vec{\gamma}}$ is a self-adjoint operator that is impossible.

It follows from the third relation in (4.8), (4.9) that

$$\sum_{j=1}^3 \gamma_j^2 = \sum_{j=1}^3 (\operatorname{Re} \gamma_j)^2 - \sum_{j=1}^3 (\operatorname{Im} \gamma_j)^2 + 2i \sum_{j=1}^3 (\operatorname{Re} \gamma_j)(\operatorname{Im} \gamma_j) > 0.$$

Hence,

$$\sum_{j=1}^3 (\operatorname{Re} \gamma_j)^2 > \sum_{j=1}^3 (\operatorname{Im} \gamma_j)^2, \quad \sum_{j=1}^3 (\operatorname{Re} \gamma_j)(\operatorname{Im} \gamma_j) = 0. \quad (4.11)$$

This means that the vectors $\operatorname{Re} \vec{\gamma}$ and $\operatorname{Im} \vec{\gamma}$ are orthogonal in \mathbb{R}^3 .

Let us fix the vector $\vec{\alpha} \in \mathbb{S}^2$ in such a way that $\vec{\alpha}$ is orthogonal to $\operatorname{Re} \vec{\gamma}$ and $\operatorname{Im} \vec{\gamma}$.

Then the standard cross product $\operatorname{Re} \vec{\gamma} \times \vec{\alpha} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \operatorname{Re} \gamma_1 & \operatorname{Re} \gamma_2 & \operatorname{Re} \gamma_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{vmatrix}$ is collinear to $\operatorname{Im} \vec{\gamma}$.

Precisely, there exists $\kappa \in \mathbb{R}$ such that

$$\operatorname{Im} \vec{\gamma} = \kappa \operatorname{Re} \vec{\gamma} \times \vec{\alpha}. \quad (4.12)$$

Calculating the norms of vectors $\operatorname{Im} \vec{\gamma}$ and $\operatorname{Re} \vec{\gamma} \times \vec{\alpha}$ in (4.12) and taking into account (4.11), we obtain

$$|\kappa|^2 = \frac{\|\operatorname{Im} \vec{\gamma}\|^2}{\|\operatorname{Re} \vec{\gamma}\|^2 \|\vec{\alpha}\|^2} = \frac{\|\operatorname{Im} \vec{\gamma}\|^2}{\|\operatorname{Re} \vec{\gamma}\|^2} = \frac{\sum_{j=1}^3 (\operatorname{Im} \gamma_j)^2}{\sum_{j=1}^3 (\operatorname{Re} \gamma_j)^2} < 1.$$

On the other hand, since $\vec{\alpha} \perp \text{Im } \vec{\gamma}$, the equation (4.10) takes the form

$$\sum_{j=1}^3 (\text{Im } \gamma_j) \sigma_j = \tanh \chi \begin{vmatrix} \sigma_1 & \sigma_2 & \sigma_3 \\ \text{Re } \gamma_1 & \text{Re } \gamma_2 & \text{Re } \gamma_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{vmatrix}. \quad (4.13)$$

Obviously, (4.13) has a solution $\chi \in \mathbb{R}$ such that $\tanh \chi = k$. Summing the results above, we prove

Theorem 4.1. *If the S -matrix $S(\cdot)$ of a non-self-adjoint operator $A_{\vec{\alpha}}$ has simple non-zero imaginary poles, then $A_{\vec{\alpha}}$ turns out to be self-adjoint with respect to new inner product $\|\cdot\|_{\text{new}}^2 = (e^{\chi Q_{\vec{\alpha}}}, \cdot)$, where $\vec{\alpha} \in \mathbb{S}^2$ is orthogonal to the vectors $\text{Re } \vec{\gamma}$, $\text{Im } \vec{\gamma}$ and χ is defined by the relation $\tanh \chi = \kappa$, where κ is the coefficient of collinearity in (4.12).*

It looks natural that the parameter χ in Theorem 4.1 correlates to the distance between imaginary poles of $S(\cdot)$.

Corollary 4.2. *Let k_{\pm} be two imaginary poles of the S -matrix of $A_{\vec{\alpha}}$. Then the parameter χ of the corresponding metric operator $e^{\chi Q_{\vec{\alpha}}}$ can be determined by the relation*

$$\cosh \chi = \frac{\|\text{Re } \vec{\gamma}\|}{|(k_- - k_+) \det \mathfrak{T}|}. \quad (4.14)$$

Proof. If k_{\pm} are poles of $S(\cdot)$, then the quantities θ_{\pm} in (2.18) are expressed as $\theta_{\pm} = 2(1 + ik_{\pm})$. Denote $\xi = \sqrt{\sum_{j=1}^3 \gamma_j^2}$. Then

$$\xi = \frac{1}{2\theta_+} - \frac{1}{2\theta_-} = i(k_- - k_+) \det \mathfrak{T}.$$

Taking into account that $\xi^2 = \sum_{j=1}^3 (\text{Re } \gamma_j)^2 - (\text{Im } \gamma_j)^2$, we obtain

$$\left\| \frac{\text{Re } \vec{\gamma}}{\xi} \right\|^2 - \left\| \frac{\text{Im } \vec{\gamma}}{\xi} \right\|^2 = 1.$$

Therefore, there exists $\omega \geq 0$ such that $\cosh \omega = \left\| \frac{\text{Re } \vec{\gamma}}{\xi} \right\|$ and $\sinh \omega = \left\| \frac{\text{Im } \vec{\gamma}}{\xi} \right\|$.

It follows from (4.12) and Theorem 4.1 that

$$|\tanh \chi| = |k| = \frac{\|\text{Im } \vec{\gamma}\|}{\|\text{Re } \vec{\gamma}\|} = \frac{\sinh \omega}{\cosh \omega} = \tanh \omega.$$

Without loss of generality¹ we can suppose that $k \geq 0$ in (4.12). Then $\chi = \omega$ and $\cosh \chi$ is determined by (4.14). ■

5. Spectral singularities

If $A_{\vec{\alpha}}$ is a self-adjoint operator in $L_2(\mathbb{R})$ or $A_{\vec{\alpha}}$ is similar to a self-adjoint one, then the entries of the S -matrix $S(k)$ are uniformly bounded when k runs \mathbb{R} . Since the existence of spectral singularity $z = k_0^2$ of $A_{\vec{\alpha}}$ should mean that $A_{\vec{\alpha}}$ cannot be similar to a self-adjoint operator, it is natural to suppose that $S(k)$ cannot be uniformly bounded in a neighborhood of $k_0 \in \mathbb{R}$. This leads to the following

¹) by choosing an appropriate direction of $\vec{\alpha}$ in (4.12)

Definition 5.1. A nonnegative number $z = k_0^2$ is called the spectral singularity of $A_{\mathfrak{T}}$ if $k_0 \in \mathbb{R}$ is a pole of the S -matrix $S(\cdot)$ of $A_{\mathfrak{T}}$. The operator $A_{\mathfrak{T}}$ has spectral singularity at infinity if $k_0 = \infty$ is a pole of $S(\cdot)$.

It is known (see, e.g. [10]) that the continuous spectrum of operators $A_{\mathfrak{T}}$ defined by (2.6) coincides with $[0, \infty)$ and there are no eigenvalues of $A_{\mathfrak{T}}$ embedded in continuous spectrum. Therefore, spectral singularities of $A_{\mathfrak{T}}$ may appear on the continuous spectrum only and (possible) existence of a spectral singularity z does not mean that z is an eigenvalue $A_{\mathfrak{T}}$.

Proposition 5.2. The operators $A_{\mathfrak{T}}$ and $A_{\mathfrak{T}}^*$ have the same set of spectral singularities.

Proof. Follows immediately from the relation $A_{\mathfrak{T}}^* = A_{\mathfrak{T}}^*$ and (3.11). ■

The existence of spectral singularity of $A_{\mathfrak{T}}$ can be easily described via the roots of the polynomial $p_{\mathfrak{T}}(k)$ defined by (3.3).

Proposition 5.3. Assume that $\mathfrak{T} \neq \frac{1}{2}\sigma_0$. A point $z = k_0^2$ is a spectral singularity of $A_{\mathfrak{T}}$ if and only if the polynomial (3.3) has:

- (i) a root $k_0 \in \mathbb{R}$ for the case of nonzero spectral singularity $z \neq 0$;
- (ii) a root $k_0 = 0$ of multiplicity 2 for the case of zero spectral singularity $z = 0$;
- (iii) no roots for the case of spectral singularity at $z = \infty$.

Proof. Let $z = k_0^2 \neq 0$ be a spectral singularity of $A_{\mathfrak{T}}$. Then $k_0 \in \mathbb{R} \setminus \{0\}$ is a pole of $S(k)$. Assume firstly that $\det \mathfrak{T} \neq 0$. Then $S(\cdot)$ is determined by (2.19), where $\theta_- \theta_+ \neq 0$ and $\theta_- \theta_+ \neq \infty$ due to the third relation in (2.18). The existence of pole k_0 of $S(\cdot)$ means that $\theta_{k_0} = 2(1 + ik_0)$ coincides with θ_- or with θ_+ . Then the point k_0 is a root of $p_{\mathfrak{T}}(k)$ due to (2.17). Conversely, if k_0 is a root of $p_{\mathfrak{T}}(k)$, then k_0 is a pole of $S(k)$ (this implication follows from (2.17) – (2.21)).

Assume now that $\det \mathfrak{T} = 0$. Then $S(\cdot)$ is determined by (2.22). The pole k_0 of $S(\cdot)$ is possible where $-2\theta_{k_0}\gamma_0 + 1 = -4(1 + ik_0)\gamma_0 + 1 = 0$. Thus, k_0 is a root of $p_{\mathfrak{T}}(k)$. Conversely statement is evident. Implication (i) is proved.

Let $z = k_0^2 = 0$ be a spectral singularity of $A_{\mathfrak{T}}$. Then $k_0 = 0$ is a pole of $S(k)$. Let $\det \mathfrak{T} \neq 0$. Then the S -matrix is determined by (2.19) and simple analysis of (2.19) shows that $S(k)$ has a pole at $k_0 = 0$ in the case $\theta_- = \theta_+ = \theta_0 = 2$ only. By (2.17), $k_0 = 0$ is a root of $p_{\mathfrak{T}}(k)$ of multiplicity 2. Conversely, let $k_0 = 0$ be a root of $p_{\mathfrak{T}}(k)$ of multiplicity 2. Then $\theta_- = \theta_+ = \theta_0 = 2$. Using (2.19) again we deduce that $S(k)$ has a pole at $k_0 = 0$. (The case $\gamma_0 = \frac{1}{2}$ and $\gamma_1 = \gamma_2 = \gamma_3 = 0$ is not considered here because, $\mathfrak{T} \neq \frac{1}{2}\sigma_0$ by the assumption of Proposition 5.3.)

Assume now that $\det \mathfrak{T} = 0$. Then $S(\cdot)$ is determined by (2.22) and this expression does not have a pole at $k_0 = 0$. On the other hand, $k_0 = 0$ cannot be a root of $p_{\mathfrak{T}}(k)$ of multiplicity 2 when $\det \mathfrak{T} = 0$. Implication (ii) is proved.

To prove (iii) it suffices to note that $S(k)$ will tend to infinity when $k \rightarrow \infty$ only in the case where $p_{\mathfrak{T}}(k)$ does not depend on k . This means that $p_{\mathfrak{T}}(k)$ has no roots in \mathbb{C} . Proposition 5.3 is proved. ■

The ‘exceptional’ operator $A_{\frac{1}{2}\sigma_0}$ in Proposition 5.3 coincides with the Krein extension of the symmetric operator A_s (see Remark 2.2).

In the particular case where $A_{\mathfrak{T}} = A_{\mathbf{T}}$, spectral singularities are described via the roots of the polynomial

$$p_{\mathbf{T}}(k) = 2dk^2 + i(\det \mathbf{T} - 4)k + 2a. \quad (5.1)$$

Corollary 5.4 ([12]). *A point $z = k_0^2$ is a spectral singularity of $A_{\mathbf{T}}$ if and only if the polynomial (5.1) has:*

- (i) a real root $k_0 \in \mathbb{R}$ for the case of nonzero spectral singularity $z \neq 0$;
- (ii) the zero root $k_0 = 0$ of multiplicity 2 for the case of spectral singularity at $z = 0$;
- (iii) no roots for the case of spectral singularity at $z = \infty$.

Proof. First of all we note that the domain of definition of $A_K (= A_{\frac{1}{2}\sigma_0})$ cannot be presented in the form (2.4). Thus $A_{\frac{1}{2}\sigma_0}$ cannot be realized as $A_{\mathbf{T}}$. Taking the expressions of γ_0 and $\det \mathfrak{T}$ given by (2.23) and (2.24) into account, we get $p_{\mathfrak{T}}(k) = \frac{1}{\Xi} p_{\mathbf{T}}(k)$. This relation and Proposition 5.3 complete the proof. ■

Proposition 5.5. *If $A_{\mathfrak{T}}$ has a spectral singularity, then $A_{\mathfrak{T}}$ can not be similar to a self-adjoint operator.*

Proof. The resolvent of an arbitrary self-adjoint operator H satisfies the inequality $\|(H - zI)^{-1}\| \leq \frac{1}{|\operatorname{Im} z|}$ for all $z \in \mathbb{C} \setminus \mathbb{R}$. If A is similar to a self-adjoint operator (i.e., (3.1) holds), then the inequality above takes the form

$$\|(A - zI)^{-1}\| \leq \frac{C}{|\operatorname{Im} z|}, \quad C = \|Z^{-1}\| \|Z\|, \quad z \in \mathbb{C} \setminus \mathbb{R}. \quad (5.2)$$

Let $A_{\mathfrak{T}}$ be similar to a self-adjoint operator. Since A_F is self-adjoint, the relation (5.2) holds for $A_{\mathfrak{T}}$ and for A_F . Therefore,

$$\|[(A_{\mathfrak{T}} - zI)^{-1} - (A_F - zI)^{-1}]g\|^2 \leq \frac{M}{(\operatorname{Im} z)^2} \|g\|^2, \quad (5.3)$$

where M is a constant independent of $g \in L_2(\mathbb{R})$ and $z \in \mathbb{C} \setminus \mathbb{R}$.

Let us consider a particular case of (5.3) with $z = k^2$ ($k \in \mathbb{C}_+$) and $g = g_{\pm}$, where

$$g_+(x) = \begin{cases} e^{-i\bar{k}x}, & x > 0; \\ 0, & x < 0 \end{cases} \quad g_-(x) = \begin{cases} 0, & x > 0 \\ e^{i\bar{k}x}, & x < 0 \end{cases}$$

Taking into account that

$$\|g_{\pm}\|^2 = \frac{1}{2\operatorname{Im} k}, \quad (Fg_{\pm})(k) = \frac{1}{2\operatorname{Im} k}, \quad \operatorname{Im} z = 2\operatorname{Im} k \operatorname{Re} k, \quad (5.4)$$

and using Lemma 3.2 we conclude that the norm of matrix²

$$\Phi(k) = \frac{\operatorname{Re} k}{p_{\mathfrak{T}}(k)} [\mathfrak{T} - \theta_k \det \mathfrak{T} \sigma_0]$$

²⁾ the matrix is considered as an operator acting in \mathbb{C}^2

is uniformly bounded on \mathbb{C}_+ . This means that the entries of $\Phi(k)$ must be uniformly bounded when k runs \mathbb{C}_+ .

Let $A_{\mathfrak{T}}$ has a spectral singularity at $z = \infty$. Then, according to Proposition 5.3, the polynomial $p_{\mathfrak{T}}(k)$ has no roots. This is possible when $\mathbf{det} \mathfrak{T} = 0$ and $\gamma_0 = 0$. In that case $\Phi(k) = \mathbf{Re} k [\sum_{j=1}^3 \gamma_j \sigma_j]$ cannot be uniformly bounded on \mathbb{C}_+ . Hence, $A_{\mathfrak{T}}$ is not similar to a self-adjoint operator.

Let $z = 0$ be a spectral singularity. Then, $A_{\mathfrak{T}} \neq A_{\frac{1}{2}\sigma_0}$ and in view of Proposition 5.3, $p_{\mathfrak{T}}(k) = qk^2$ ($q \neq 0$ is some constant). In that case, at least one of entries of $\Phi(k) = \frac{\mathbf{Re} k}{qk^2} [\mathfrak{T} - \theta_k \mathbf{det} \mathfrak{T} \sigma_0]$ tends to infinity when $k \rightarrow 0$. So, $A_{\mathfrak{T}}$ is not similar to a self-adjoint operator.

Let $z = k_0^2$ be a non-zero spectral singularity. Then $k_0 \in \mathbb{R}$ is a root of $p_{\mathfrak{T}}(k)$ and $\Phi(k)$ tends to infinity when $k \rightarrow k_0$. Thus $A_{\mathfrak{T}}$ is not similar to a self-adjoint operator. Proposition 5.5 is proved. ■

Example IV. *δ' -potential with a complex coupling.* Let $d \in \mathbb{C}$ and $a = b = c = 0$. Then the expression

$$-\frac{d^2}{dx^2} + d < \delta', \cdot > \delta'(x), \quad d \in \mathbb{C}$$

determines the operators $A_d = -\frac{d^2}{dx^2}$ in $L_2(\mathbb{R})$, which are defined on

$$\mathcal{D}(A_d) = \left\{ f \in W_2^2(\mathbb{R} \setminus \{0\}) \mid \begin{array}{l} f'(0+) = f'(0-) \ (\equiv f'(0)) \\ f(0+) - f(0-) = -df'(0) \end{array} \right\}$$

In that case

$$\mathfrak{T} = \frac{1}{4-2d} \begin{pmatrix} 1-d & 1 \\ 1 & 1-d \end{pmatrix}, \quad \mathbf{det} \mathfrak{T} = -\frac{d}{2(4-2d)}, \quad \gamma_0 = \frac{1-d}{4-2d}.$$

Substituting these quantities in (2.16) we obtain

$$S(k) = \frac{1}{dk-2i} \begin{pmatrix} -dk & 2i \\ 2i & -dk \end{pmatrix}.$$

The S -matrix has a real pole $k_0 = \frac{2i}{d}$ when $d \in i\mathbb{R} \setminus \{0\}$. In that case $z = k_0^2 = \frac{4}{|d|^2}$ is a spectral singularity of A_d .

6. Exceptional points

Let A be a linear operator acting in a Hilbert space \mathfrak{H} . A nonzero vector $f \in \mathcal{D}(A)$ is called a *root vector* of A corresponding to the eigenvalue z if $(A - zI)^n f = 0$ for some $n \in \mathbb{N}$. The set of all roots vectors of A corresponding to a given eigenvalue z , together with zero vector, forms a linear subspace \mathcal{L}_z , which is called the *root subspace*. The dimension of the root subspace \mathcal{L}_z is called the *algebraic multiplicity*

of the eigenvalue z . The *geometric multiplicity* of z is defined as the dimension of the kernel subspace $\ker(A - zI)$ (i.e., as the dimension of the linear subspace of eigenfunctions of A corresponding to z).

The algebraic and the geometric multiplicities of z coincide in the case where A is similar to a self-adjoint operator.

The existence of exceptional points deals with the possible occurrence of nontrivial Jordan blocks in discrete spectra. For operators $A_{\mathfrak{T}}$ depending on parameters $\mathfrak{T} = \{\mathfrak{t}_{ij}\}$ this means that two eigenvalues $z_1(\mathfrak{T})$, $z_2(\mathfrak{T})$ may coalesce (degenerate) at certain parameter hypersurfaces of the linear set $\{\mathfrak{t}_{ij}\}$ under simultaneous coalescence of the corresponding eigenvectors $f_1(\mathfrak{T})$, $f_2(\mathfrak{T})$ see e.g. [2]. We formalize these ideas as follows:

Definition 6.1. *Let A be a linear operator acting in a Hilbert space \mathfrak{H} . An eigenvalue z of A is called the exceptional point if the geometric multiplicity of z does not coincide with its algebraic multiplicity.*

The presence of an exceptional point means that the operator A is not self-adjoint in \mathfrak{H} and, moreover, it cannot be self-adjoint for any choice of (equivalent) inner product of \mathfrak{H} .

Theorem 6.2. *Let $S(\cdot)$ be the S -matrix of $A_{\mathfrak{T}}$. Then $k_0 \in \mathbb{C}_+$ is a pole of order 2 of $S(\cdot)$ if and only if $z_0 = k_0^2$ is an exceptional point of $A_{\mathfrak{T}}$.*

Proof. The resolvent $(A_F - zI)^{-1}$ of a self-adjoint operator A_F (see (2.11)) is a holomorphic operator-valued function on $\mathbb{C} \setminus \mathbb{R}_+$.

On the other hand, if $A_{\mathfrak{T}}$ is defined by (2.6), then the resolvent $(A_{\mathfrak{T}} - zI)^{-1}$ may be a meromorphic function on $\mathbb{C} \setminus \mathbb{R}_+$ and an eigenvalue $z_0 = k_0^2$ of $A_{\mathfrak{T}}$ will be exceptional if and only if $(A_{\mathfrak{T}} - zI)^{-1}$ has a pole z_0 of order greater than one³ [17]. Hence, the existence of an exceptional point $z_0 = k_0^2$ of $A_{\mathfrak{T}}$ is equivalent to the existence of pole z_0 of order 2 for the operator-valued function

$$(A_{\mathfrak{T}} - zI)^{-1} - (A_F - zI)^{-1}.$$

Taking the proof of Lemma 3.2 into account (especially (3.5) and (3.7)) we conclude that this condition is equivalent to the existence of pole $k_0 \in \mathbb{C}_+$ of order 2 for the matrix-valued function $\mathfrak{T}(\sigma_0 - \theta_k \mathfrak{T})^{-1}$.

It should be noted that $z_0 = -1$ cannot be an exceptional point of $A_{\mathfrak{T}}$ (because $-1 \in \rho(A_{\mathfrak{T}})$ for any operator $A_{\mathfrak{T}}$ defined by (2.6)). Hence, the possible pole $k_0 \neq i$ and we can suppose that $\theta_k \neq 0$ in some neighbourhood of $\theta_{k_0} = 2(1 + ik_0)$. Then

$$\mathfrak{T}(\sigma_0 - \theta_k \mathfrak{T})^{-1} = -\frac{1}{\theta_k} \sigma_0 + \frac{1}{\theta_k} (\sigma_0 - \theta_k \mathfrak{T})^{-1}.$$

Comparing the obtained decomposition with (2.9) we conclude that k_0 is pole of order 2 of $\mathfrak{T}(\sigma_0 - \theta_k \mathfrak{T})^{-1}$ if and only if k_0 is pole of order 2 of the S -matrix $S(\cdot)$. Theorem 6.2 is proved. ■

³⁾ in our case, the order must be 2 because the defect indices of the symmetric operator A_s are $< 2, 2 >$

Corollary 6.3. *The point $z_0 = k_0^2$ is an exceptional point of $A_{\mathfrak{T}}$ if and only if the matrix $\sigma_0 - \theta_{k_0}\mathfrak{T}$ is nonzero and nilpotent.*

Proof. Let $z_0 = k_0^2$ be an exceptional point of $A_{\mathfrak{T}}$. Then $k_0 \in \mathbb{C}_+$ is a pole of order 2 for $S(\cdot)$. Taking (2.16) into account, we conclude that $\det \mathfrak{T} \neq 0$ and $k_0 \neq i$. So, $S(\cdot)$ is defined by (2.19) and $\theta_{k_0} = 2(1 + ik_0) \neq 0$.

The S -matrix $S(\cdot)$ has a pole k_0 of order 2 if and only if at least one of functions $s_j(\cdot)$ in the decomposition (2.20) has pole k_0 of order 2. In that case, the simple analysis of (2.21) shows that $\theta_+ = \theta_- = \theta_{k_0}$. Then, in view of (2.18),

$$\sum_{j=1}^3 \gamma_j^2 = 0, \quad \theta_+ = \theta_- = \theta_{k_0} = \frac{1}{\gamma_0}. \quad (6.1)$$

We note that not all coefficients γ_j are equal to zero in the first relation of (6.1). Indeed, suppose that $\gamma_1 = \gamma_2 = \gamma_3 = 0$. Then $\mathfrak{T} = \gamma_0 \sigma_0$ and $\theta_- \theta_+ = 1/\gamma_0^2$. Substituting these quantities into (2.19), we obtain

$$S(k) = \left[1 - \frac{4ik}{\theta_k - 1/\gamma_0} \right] \sigma_0 = -\frac{k + k_0}{k - k_0} \sigma_0.$$

Therefore, k_0 cannot be a pole of order 2. The obtained contradiction means that at least one of coefficients $\gamma_1, \gamma_2, \gamma_3$ differs from zero. In that case, the matrix

$$\sigma_0 - \theta_{k_0}\mathfrak{T} = (1 - \theta_{k_0}\gamma_0)\sigma_0 - \theta_{k_0} \sum_{j=1}^3 \gamma_j \sigma_j = -\theta_{k_0} \sum_{j=1}^3 \gamma_j \sigma_j$$

is nonzero.

On the other hand, taking (6.1) and properties of Pauli matrices into account,

$$(\sigma_0 - \theta_{k_0}\mathfrak{T})^2 = \theta_{k_0}^2 \left(\sum_{j=1}^3 \gamma_j \sigma_j \right)^2 = \theta_{k_0}^2 \left(\sum_{j=1}^3 \gamma_j^2 \right) \sigma_0 = 0.$$

Conversely, let $\sigma_0 - \theta_{k_0}\mathfrak{T}$ be a nonzero and nilpotent matrix. In that case

$$\sigma_0 - \theta_{k_0}\mathfrak{T} = (1 - \theta_{k_0}\gamma_0)\sigma_0 - \theta_{k_0} \sum_{j=1}^3 \gamma_j \sigma_j \neq 0$$

and

$$\begin{aligned} 0 &= (\sigma_0 - \theta_{k_0}\mathfrak{T})^2 = \left[(1 - \theta_{k_0}\gamma_0)\sigma_0 - \theta_{k_0} \sum_{j=1}^3 \gamma_j \sigma_j \right]^2 = \\ &= [(1 - \theta_{k_0}\gamma_0)^2 + \theta_{k_0}^2 \sum_{j=1}^3 \gamma_j^2] \sigma_0 + 2(1 - \theta_{k_0}\gamma_0)\theta_{k_0} \sum_{j=1}^3 \gamma_j \sigma_j. \end{aligned}$$

These relations are possible only in the case: $1 - \theta_{k_0}\gamma_0 = 0$ and $\sum_{j=1}^3 \gamma_j^2 = 0$, where at least one γ_j differs from zero. Then $\theta_{k_0} = \theta_+ = \theta_- = \frac{1}{\gamma_0}$ and $k_0 = i - \frac{i}{2\gamma_0}$ is a pole of order 2 of $S(\cdot)$. Corollary 6.3 is proved. ■

In the particular case where $A_{\mathfrak{T}} = A_{\mathbf{T}}$, the (possible) appearance of exceptional point is determined by parameters a, d .

Corollary 6.4. *Let $z_0 = k_0^2$ be an exceptional point of $A_{\mathbf{T}}$. Then*

$$k_0 = -i \frac{4 - \det \mathbf{T} + 4a}{4 - \det \mathbf{T} - 4d} = i \frac{4 - \det \mathbf{T}}{4d} \quad (6.2)$$

and $z = k_0^2 = \frac{a}{d}$.

Proof. If $z_0 = k_0^2$ is an exceptional point of $A_{\mathbf{T}}$, then $k_0 \in \mathbb{C}_+$ is a pole of order 2 of $S(\cdot)$. Then $k_0 = i - \frac{i}{2\gamma_0}$ and the first relation in (6.2) follows from (2.23).

Using (2.24), (6.1) and taking into account that

$$(4 - \det \mathbf{T})^2 + 16ad = (4 - ad + bc)^2 + 16ad = (4 + ad - bc)^2 + 16bc = (4 + \det \mathbf{T})^2 + 16bc$$

we conclude that $(4 - \det \mathbf{T})^2 + 16ad = 0$. Therefore,

$$k_0 = -i \frac{4 - \det \mathbf{T} + 4a}{4 - \det \mathbf{T} - 4d} = -i \frac{4 - \det \mathbf{T} + 4a}{4 - \det \mathbf{T} - 4d} \cdot \frac{4 - \det \mathbf{T} + 4d}{4 - \det \mathbf{T} + 4d} = i \frac{4 - \det \mathbf{T}}{4d}.$$

To complete the proof it suffices to calculate

$$z = k_0^2 = -\frac{(4 - \det \mathbf{T})^2}{16d^2} = \frac{16ad}{16d^2} = \frac{a}{d}.$$

■

The S-matrices in Examples I-IV do not have poles of order 2. Hence, the corresponding operators $A_{\tilde{\mathbf{x}}}$ do not have exceptional points.

Example V. Let $a = -e^{i\phi}$, $b = -1$, $c = 1$, and $d = e^{-i\phi}$. Then (2.1) takes the form

$$-\frac{d^2}{dx^2} - e^{i\phi} < \delta, \cdot > \delta(x) - < \delta', \cdot > \delta(x) + < \delta, \cdot > \delta'(x) + e^{-i\phi} < \delta', \cdot > \delta'(x)$$

and (2.4) determines the operators $A_\phi = -\frac{d^2}{dx^2}$ with domains of definition

$$\mathcal{D}(A_\phi) = \left\{ f \in W_2^2(\mathbb{R} \setminus \{0\}) \mid \begin{array}{l} f(0+) + e^{-i\phi} f'(0+) = 2f(0-) \\ f(0-) = e^{-i\phi} f'(0-) \end{array} \right\}.$$

If $\phi \in (0, 2\pi)$, then $\mathcal{D}(A_\phi)$ can be presented in the form (2.6), where

$$\mathfrak{T} = \frac{1}{8 \sin^2 \phi/2} \begin{pmatrix} 1 - e^{-i\phi} & 2 \\ 0 & 1 - e^{-i\phi} \end{pmatrix}.$$

In that case

$$\theta_- = \theta_+ = 2(1 - e^{i\phi}), \quad \det \mathfrak{T} = \frac{1}{4(1 - e^{i\phi})} \neq 0.$$

Substituting these quantities in (2.19) we obtain

$$S(k) = -\frac{k + ie^{i\phi}}{k - ie^{i\phi}} \sigma_0 + \frac{2ik}{(k - ie^{i\phi})^2} \begin{pmatrix} 0 & 2e^{i\phi} \\ 0 & 0 \end{pmatrix}.$$

The S -matrix has pole $k_0 = ie^{i\phi}$ of order 2 in the physical sheet \mathbb{C}_+ when $\phi \in [0, \frac{\pi}{2}) \cup (\frac{3\pi}{2}, 2\pi]$. In that case $z_0 = -e^{2i\phi}$ is the exceptional point of A_ϕ .

If ϕ coincides with $\frac{\pi}{2}$ or with $\frac{3\pi}{2}$, then the S -matrix has real poles $k_0 = -1$ or $k_0 = 1$, respectively. The operator A_ϕ has spectral singularity $z_0 = 1$.

If $\phi \in (\frac{\pi}{2}, \frac{3\pi}{2})$, then the pole k_0 of the S -matrix belongs to the nonphysical sheet \mathbb{C}_- . The corresponding operator A_ϕ is similar to self-adjoint.

7. Conclusions

This paper shows that poles of S -matrix $S(\cdot)$ completely characterize the properties of Schrödinger operators $A_{\mathfrak{T}}$ with non-symmetric zero-range potentials (2.2). Precisely, poles of $S(\cdot)$ on the physical sheet \mathbb{C}_+ describe the discrete spectrum σ_p of $A_{\mathfrak{T}}$. The appearance of exceptional points on σ_p is distinguished by poles of order 2 on the physical sheet. The existence of spectral singularities on the continuous spectrum σ_c of $A_{\mathfrak{T}}$ is determined by poles of $S(\cdot)$ on the extended real line $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. The property of similarity of $A_{\mathfrak{T}}$ to a self-adjoint operator means that the S -matrix $S(\cdot)$ has poles in the nonphysical sheet \mathbb{C}_- or $S(\cdot)$ has simple non-zero imaginary poles.

Not every operator $A_{\mathfrak{T}}$ defined by (2.6) and studied in the paper can be interpreted as pseudo-hermitian or \mathcal{PT} -symmetric. Sometimes [18], such more general class of operators is called *quasi-self-adjoint*. Our studies show that techniques based on the decomposition of S -matrix with respect to the Pauli matrices have proved very useful for investigation of quasi-self-adjoint operators. In this way, we find an explicit expression of metric operators for the case where S -matrix has simple non-zero imaginary poles.

The results of the paper were established with the use of expression (2.9) for S -matrices which comes from the Lax-Phillips scattering theory and it is closed to the concept of characteristic function of quasi-self-adjoint operators [18]. Using the equivalent representation (2.28) of the S -matrix we can reformulate the obtained results in terms of reflection and transmission coefficients.

The methods developed in the paper can be applied for studies of S -matrices of Schrödinger operators with non-symmetric potentials having a compact support.

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